

# IX Workshop on novel methods for electronic structure calculation

## Theoretical-computational study of $\text{CsGeX}_3$ ( $X = \text{Cl}, \text{Br}, \text{I}$ ) perovskites and their applications for solar cells

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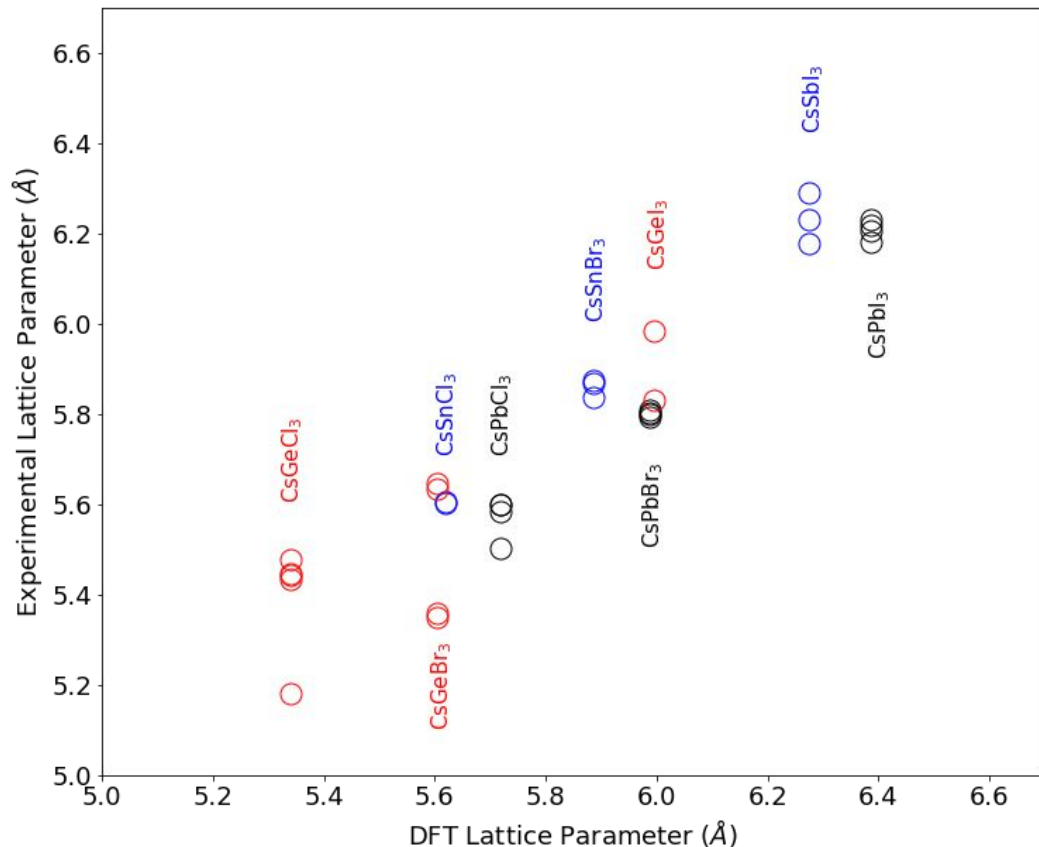
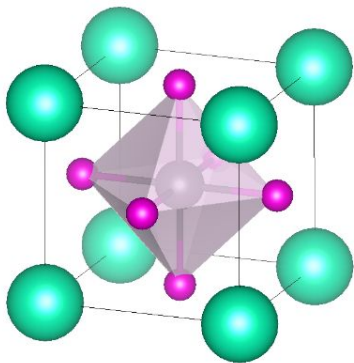


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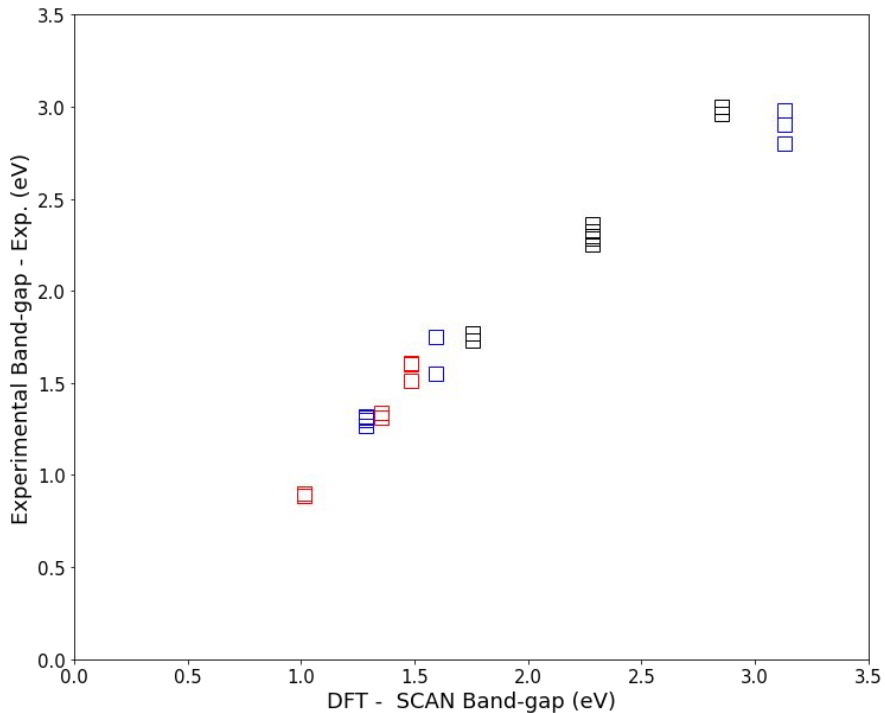
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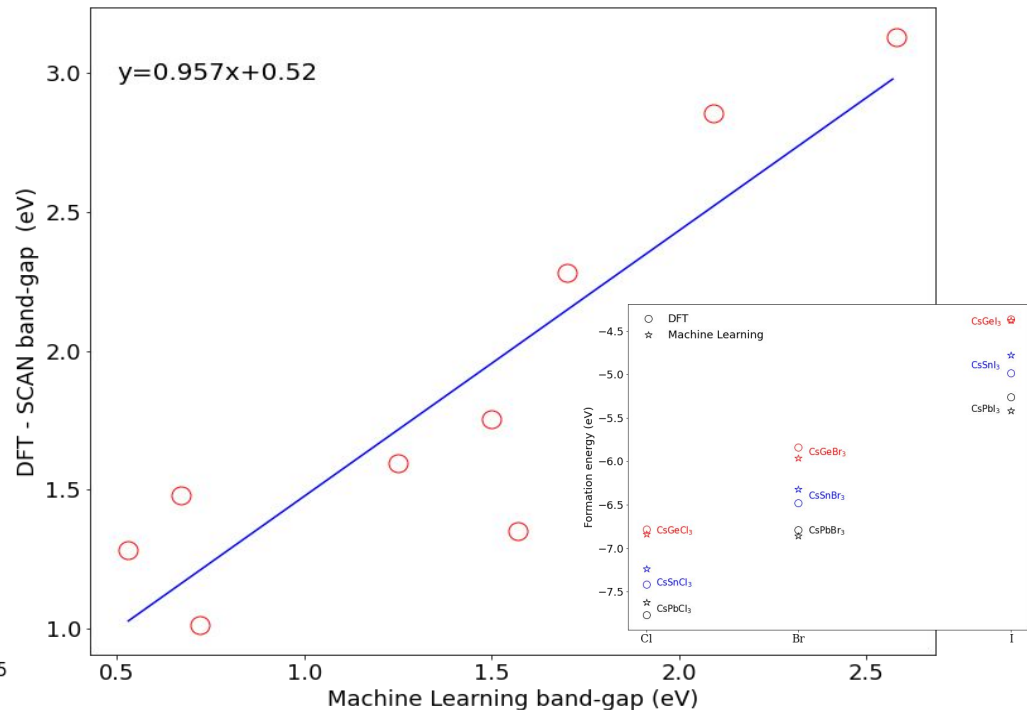
- Ab-initio calculations based on the Density Functional Theory, using the Full-Potential Linearized Augmented Plane-Wave method (FP-LAPW), implemented in the ELK code.
- Exchange-Correlation: meta-GGA SCAN.
- A grid of 13x13x13 k-point to sample the reciprocal space.
- Crystal structure with space group Pm-3m



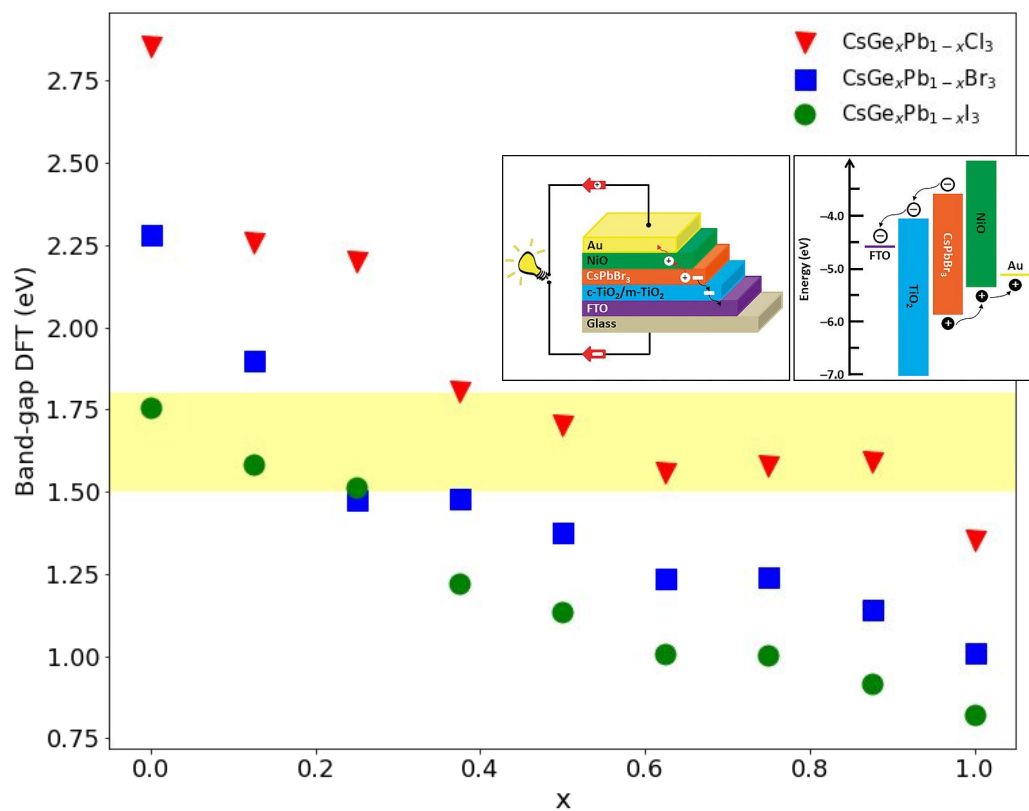
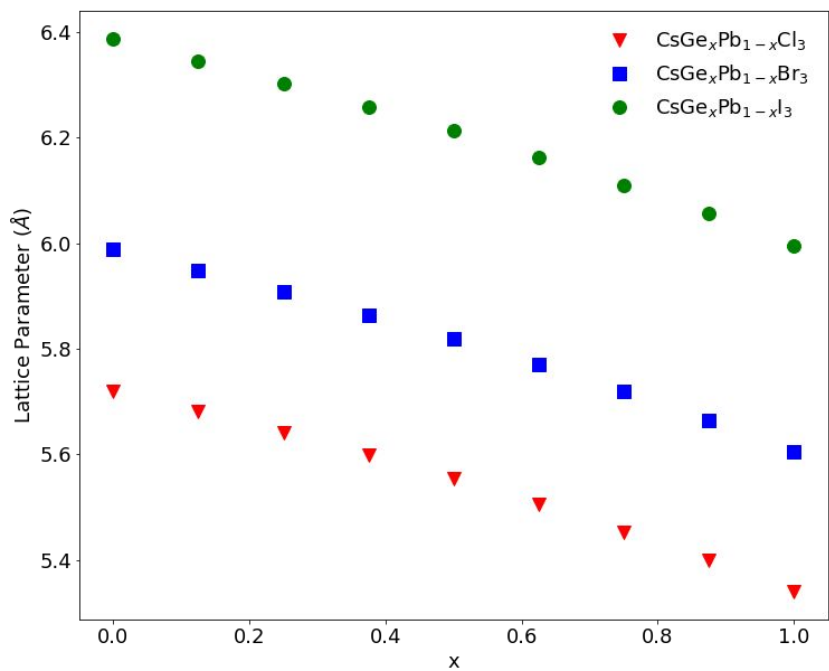
## Band-gap: DFT - SCAN, Machine Learning and experimental data



Good agreement between DFT-SCAN results and experimental data



Linear relation between DFT-SCAN and machine learning values



- New Pb-free compounds to use in the design of perovskite-based solar cells.
- DFT and Machine Learning methodologies to search new compounds.
- Accurate results of DFT compared with experimental ones.

- Based in these results, the next step is the design of the solar cell device using SCAPS 1D Simulations, and try to synthesize these solar cells.